LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009457.D
Acq On : 30 Mar 2017 18:57
Operator : SJ/MA
Sample : I2446-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.375	214	219	225	rBV	112967	159006	1.73%	0.387%
2	4.969	315	320	331	rBV	633839	876039	9.52%	2.130%
3	5.422	391	397	407	rBV	913096	1323480	14.38%	3.218%
4	6.040	496	502	510	rBV	113693	167539	1.82%	0.407%
5	7.004	660	666	677	rVB	527394	841720	9.15%	2.047%
6	7.381	723	730	737	rBV	1590893	2523964	27.43%	6.137%
7	7.851	803	810	816	rBV	506085	813674	8.84%	1.978%
8	8.169	855	864	872	rBV	2310579	3655526	39.73%	8.888%
9	9.016	999	1008	1018	rBV	1982797	3252472	35.35%	7.908%
10	10.645	1278	1285	1293	rBV	619792	1027642	11.17%	2.499%
11	13.110	1696	1704	1712	rBV	4513077	6415292	69.72%	15.599%
12	13.945	1840	1846	1852	rBV	124184	165480	1.80%	0.402%
13	14.492	1933	1939	1950	rVB3	841557	1253886	13.63%	3.049%
14	15.986	2187	2193	2203	rBV	2088171	3047015	33.12%	7.409%
15	16.186	2222	2227	2234	rBV	72418	130148	1.41%	0.316%
16	17.239	2400	2406	2414	rBV	1052617	1526470	16.59%	3.712%
17	18.115	2549	2555	2559	rBV	121377	166950	1.81%	0.406%
18	19.392	2768	2772	2781	rBV4	82574	127542	1.39%	0.310%
19	19.862	2845	2852	2858	rBV	7411688	9201072	100.00%	22.372%
20	21.103	3059	3063	3069	rBV	206780	268843	2.92%	0.654%
21	21.415	3111	3116	3121	rBV	1816905	2111735	22.95%	5.135%
22	23.738	3504	3511	3519	rBV	1031591	2071213	22.51%	5.036%

Sum of corrected areas: 41126708

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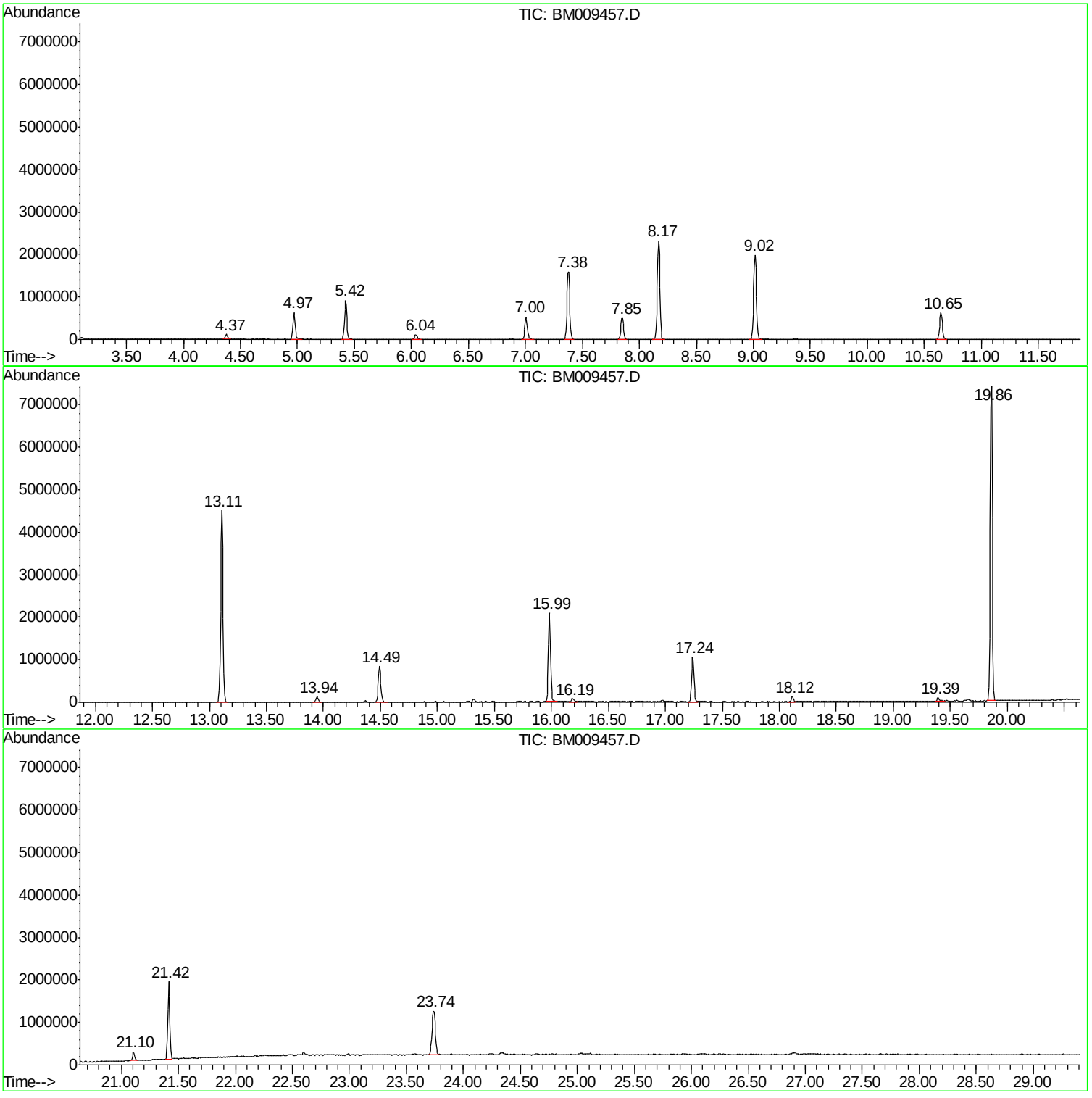
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009457.D
Acq On : 30 Mar 2017 18:57
Operator : SJ/MA
Sample : I2446-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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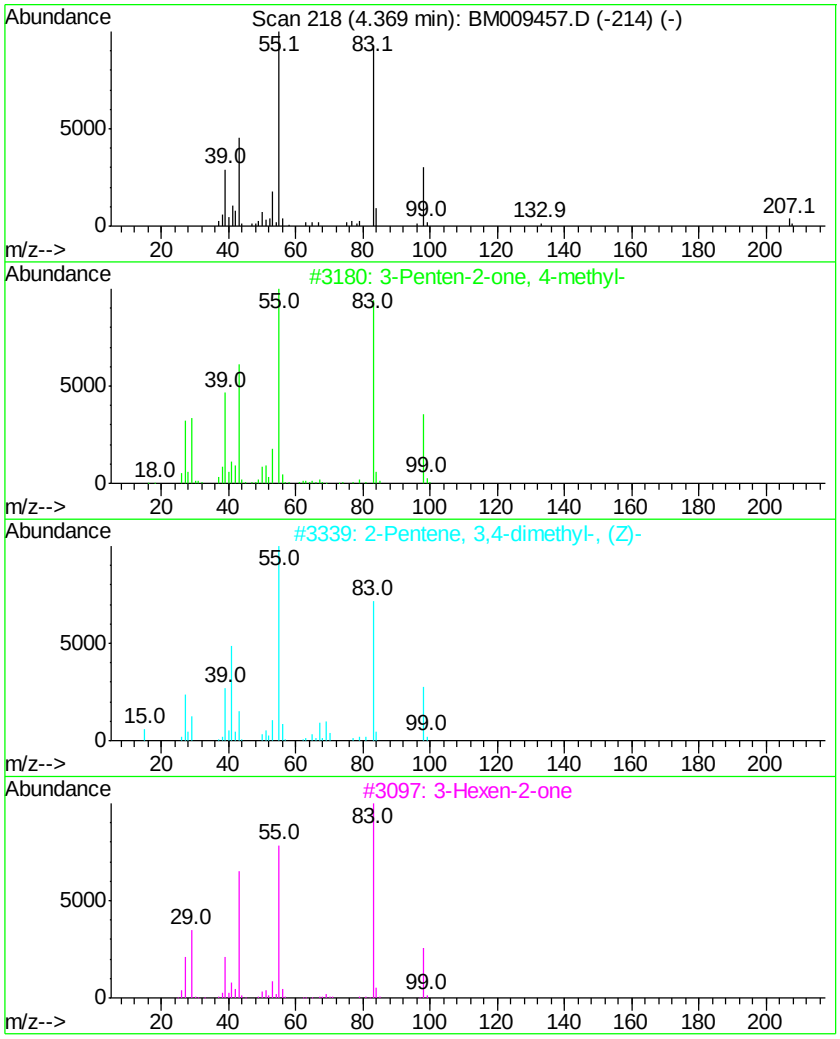
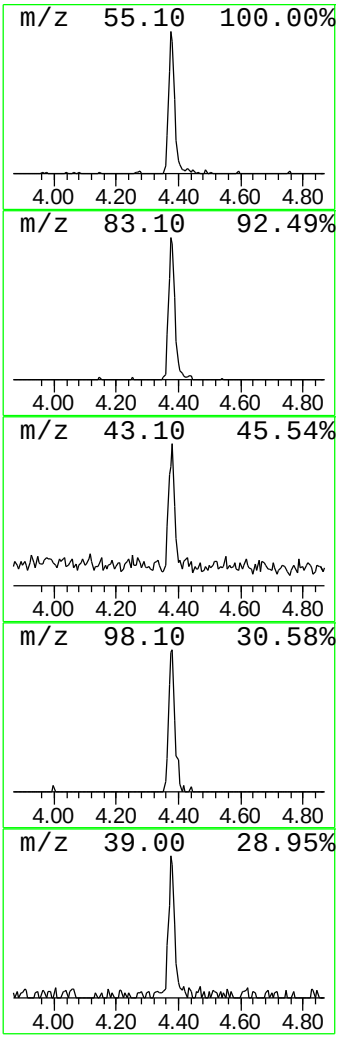
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	3.91 ng	159006	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
3	3-Hexen-2-one	98	C6H10O	000763-93-9	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	80





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Misc :
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Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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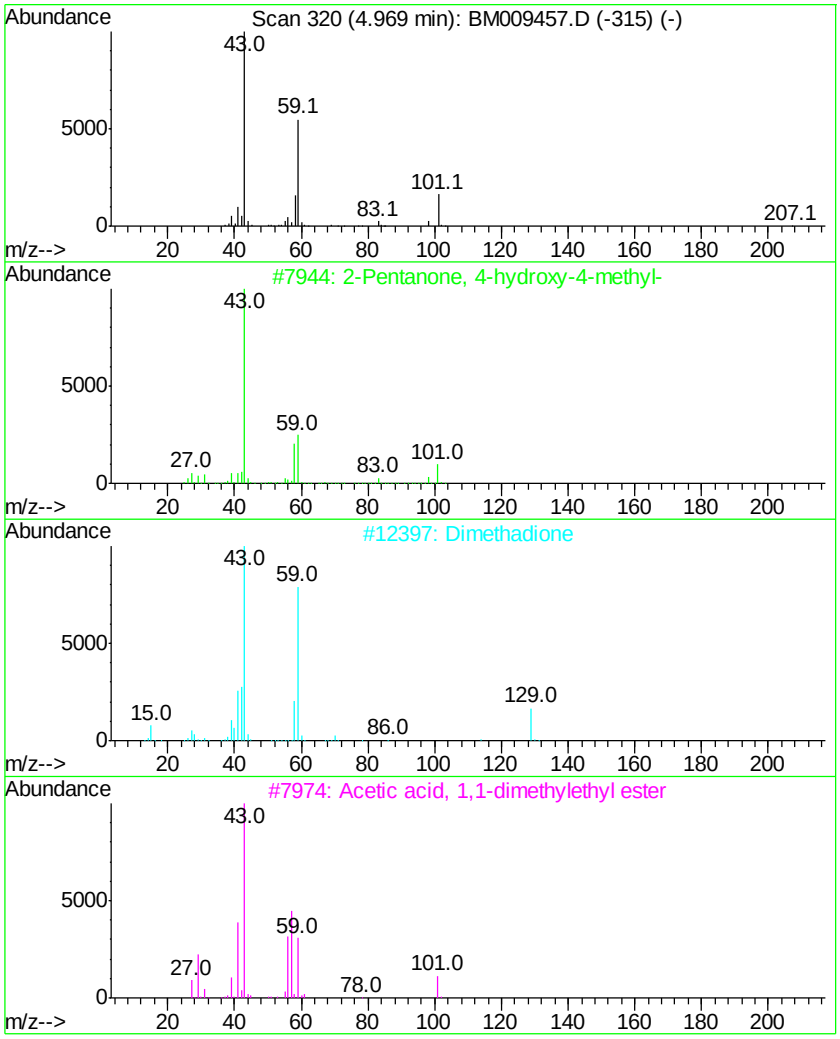
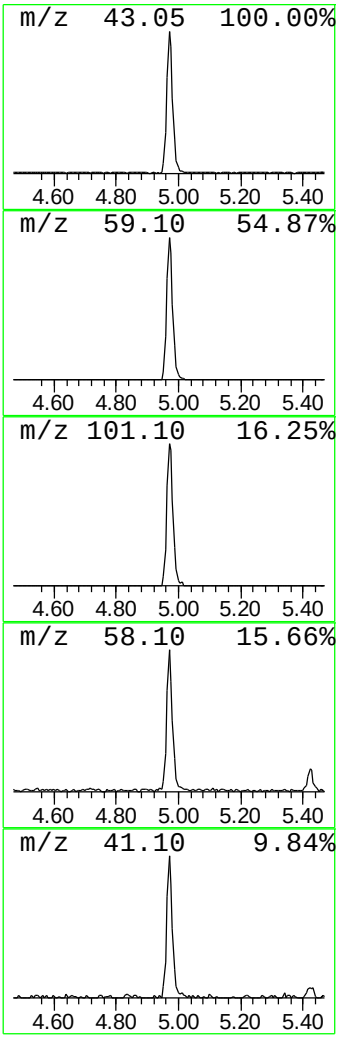
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	21.53 ng	876039	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Dimethadione	129	C5H7NO3	000695-53-4	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BM009457.D
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Operator : SJ/MA
Sample : I2446-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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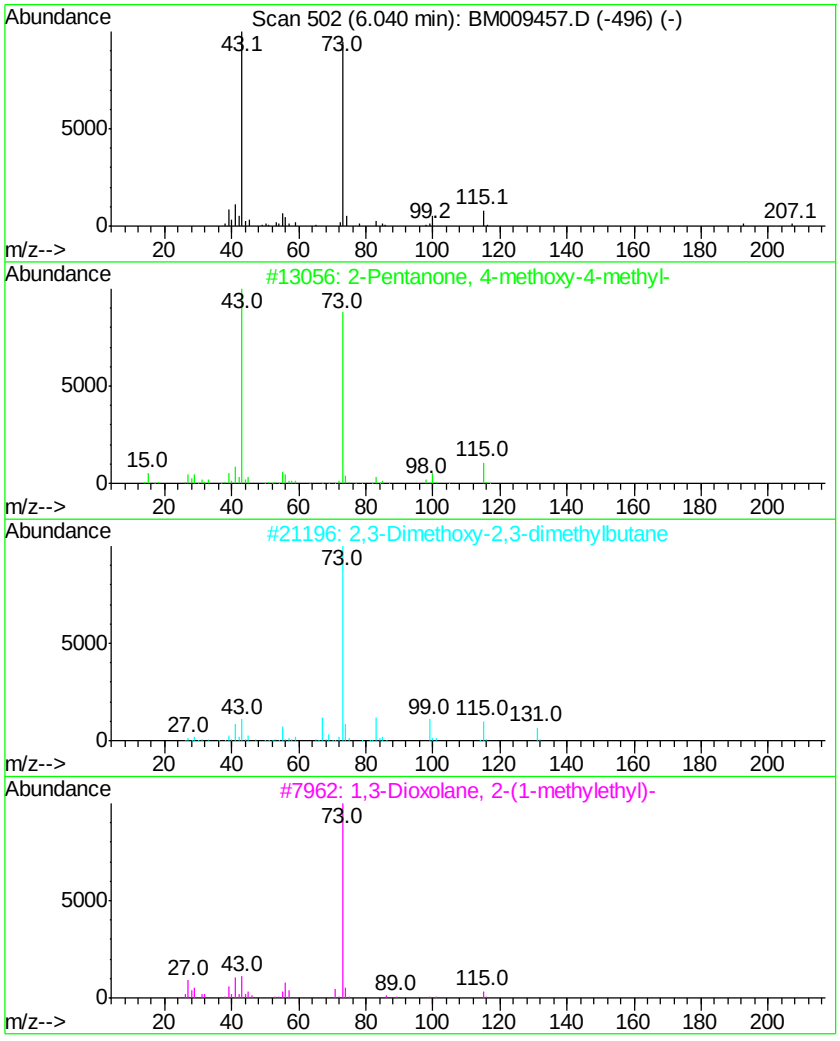
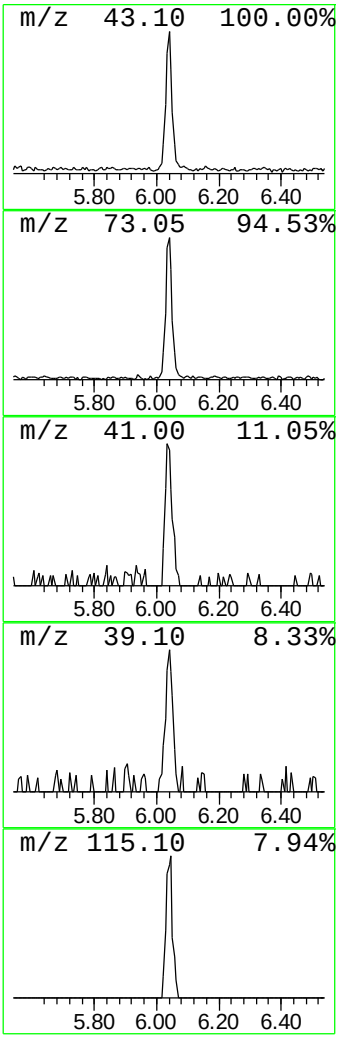
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	4.12 ng	167539	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	2,3-Dimethoxy-2,3-dimethylbutane	146	C8H18O2	006091-59-4	23
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4	3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	10
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : I2446-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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TIC Library : C:\DATABASE\NIST02.L
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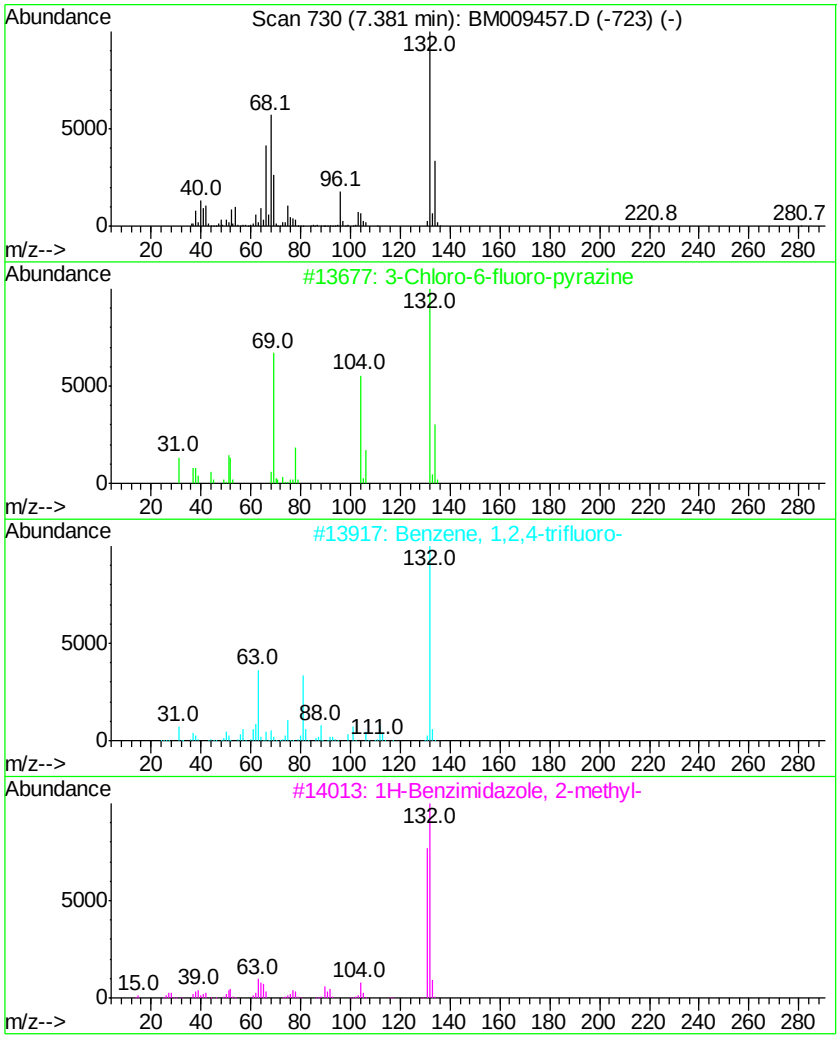
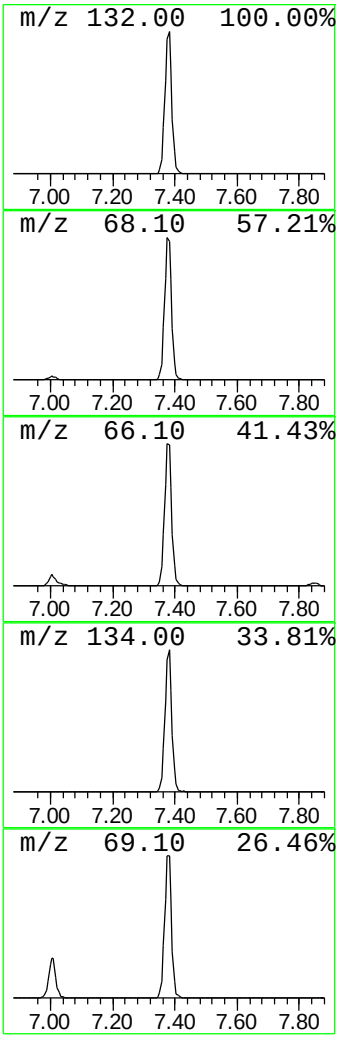
Peak Number 4 unknown7.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	62.04 ng	2523960	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1,1-Difluoro-3-methyl-1-silacycl...	134	C5H8F2Si	054077-66-6	9





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Sample : I2446-01
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Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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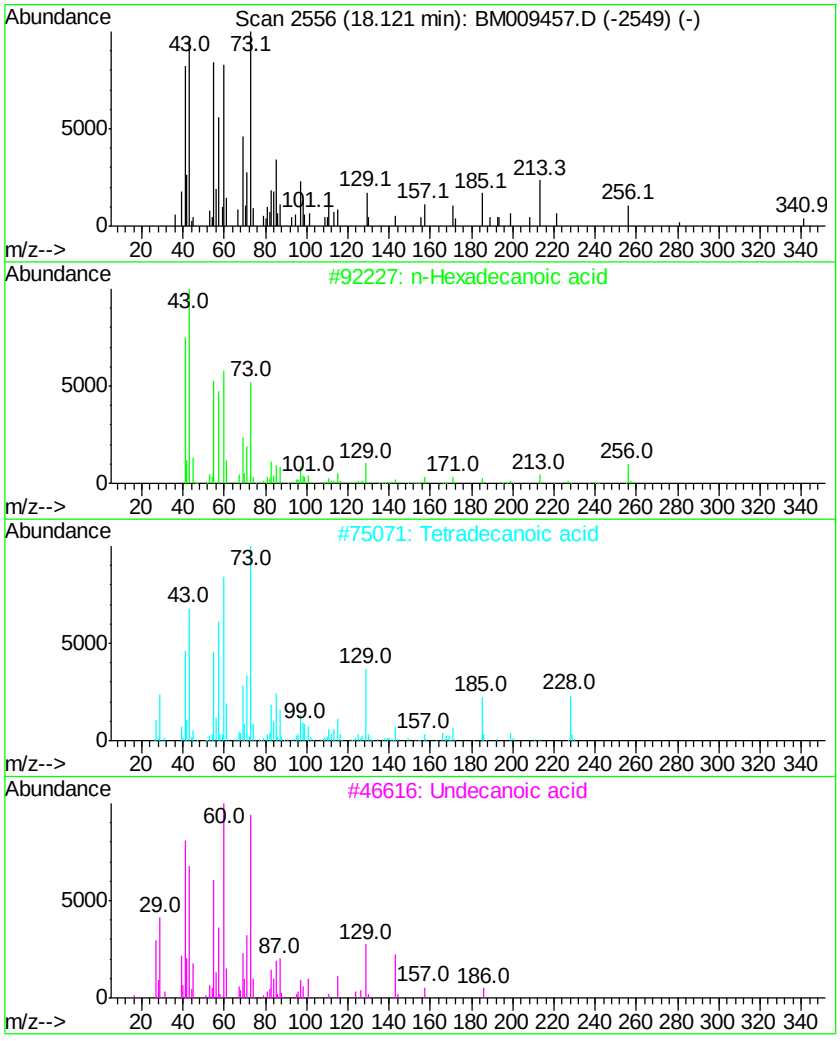
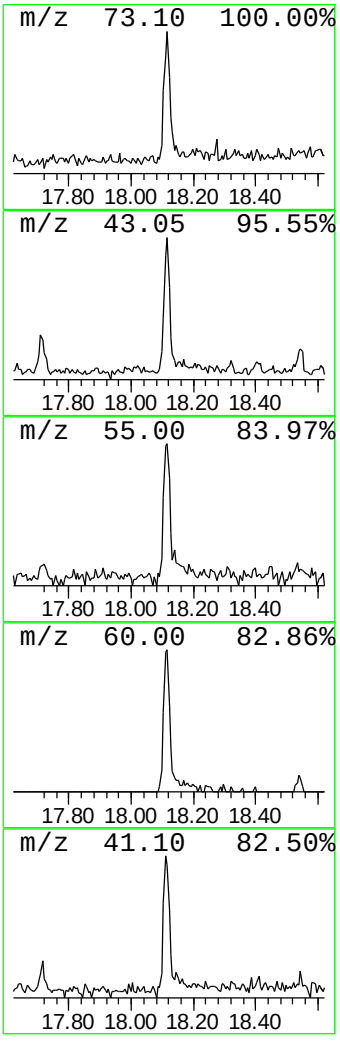
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	2.19 ng	166950	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	62
5	D-Glucopyranoside, 4-O-decyl-	320	C16H32O6	1000158-00-4	47





Library Search Compound Report

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Operator : SJ/MA
Sample : I2446-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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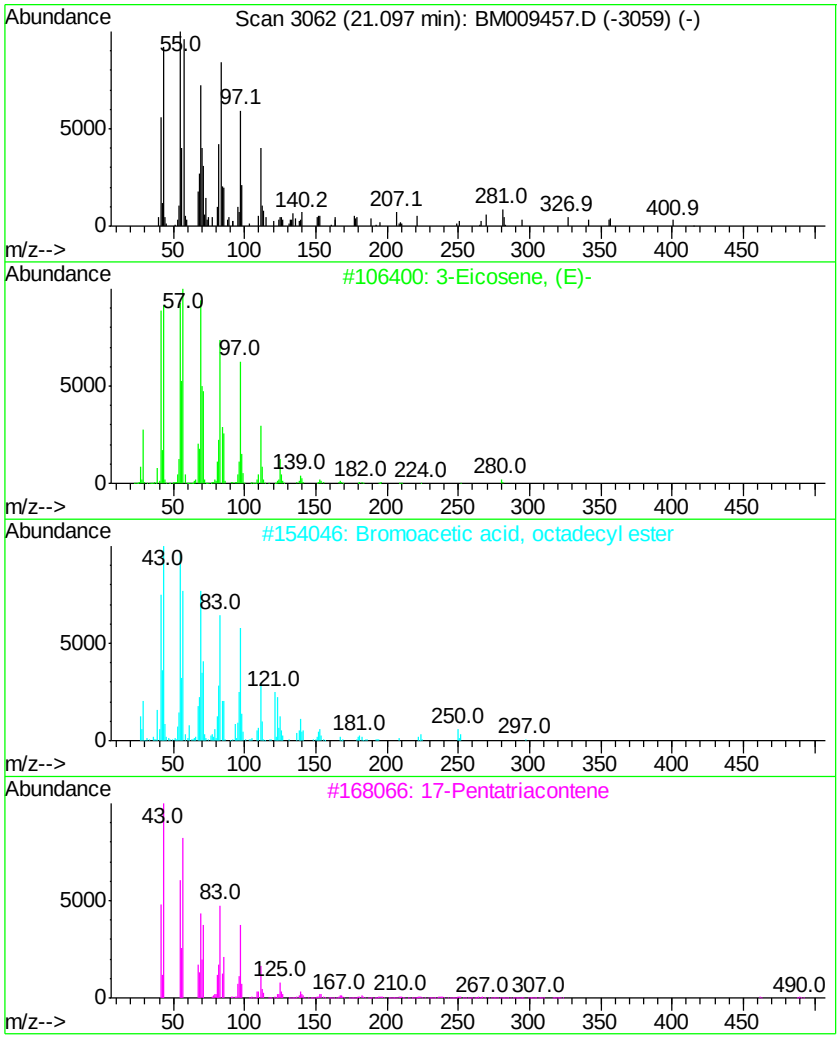
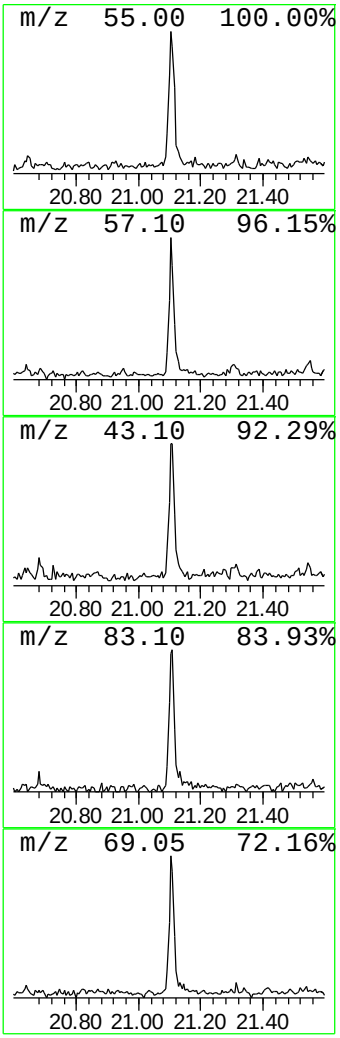
Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.55 ng	268843	Chrysene-d12	21.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	80
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	72
5	1-Docosanol	326	C22H46O	000661-19-8	70





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.37	3.9	ng	159006	1	7.85	813674	20.0
2-Pentanone, 4-hy...	4.97	21.5	ng	876039	1	7.85	813674	20.0
2-Pentanone, 4-me...	6.04	4.1	ng	167539	1	7.85	813674	20.0
unknown7.38	7.38	62.0	ng	2523960	1	7.85	813674	20.0
n-Hexadecanoic acid	18.12	2.2	ng	166950	4	17.24	1526470	20.0
3-Eicosene, (E)-	21.10	2.5	ng	268843	5	21.42	2111740	20.0